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High-Performance Computational Modeling for Tight Budgets

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A new generation of high-performance scientific software and working methods is appearing in today's marketplace. Recent advances in general-purpose software for solving Partial Differential Equations (*PDE's*) now enable a greater number of technical users to develop sophisticated numerical computer models for solving diverse problems, without the large investments previously needed for programming, numerical algorithms, and code maintenance in each significant project. In much the same way that authors today use "word processors" without knowing the internal software logic and programming details, scientists and engineers can use emerging "modeling processors" to simulate complex physical processes.

This article presents results of testing and practical experience with the high-performance software system, *PDEase*. Symbolic processing techniques in this system translate physical problem statements into efficient computer models. Internal details of mesh generation, adaptive grid refinement, linear system solution, nonlinear solution techniques, and error estimation are all provided automatically by the software package. Flexible graphical output is also provided so that, in most cases, a full model can be specified in a single page of input. When needed for special-purpose applications, additions to the core package have been made with modest effort.

The present use of *PDEase* was motivated by needs to simultaneously economize and enhance flow and transport modeling performance in the Superfund cleanup of contaminated ground water at the DOE/LLNL Livermore site. We describe applications to both forward and inverse flow problems that are encountered in regulatory-driven remedial designs and compliance monitoring evaluations. Other applications, showing the range of problems accessible to the software, will also be described.

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